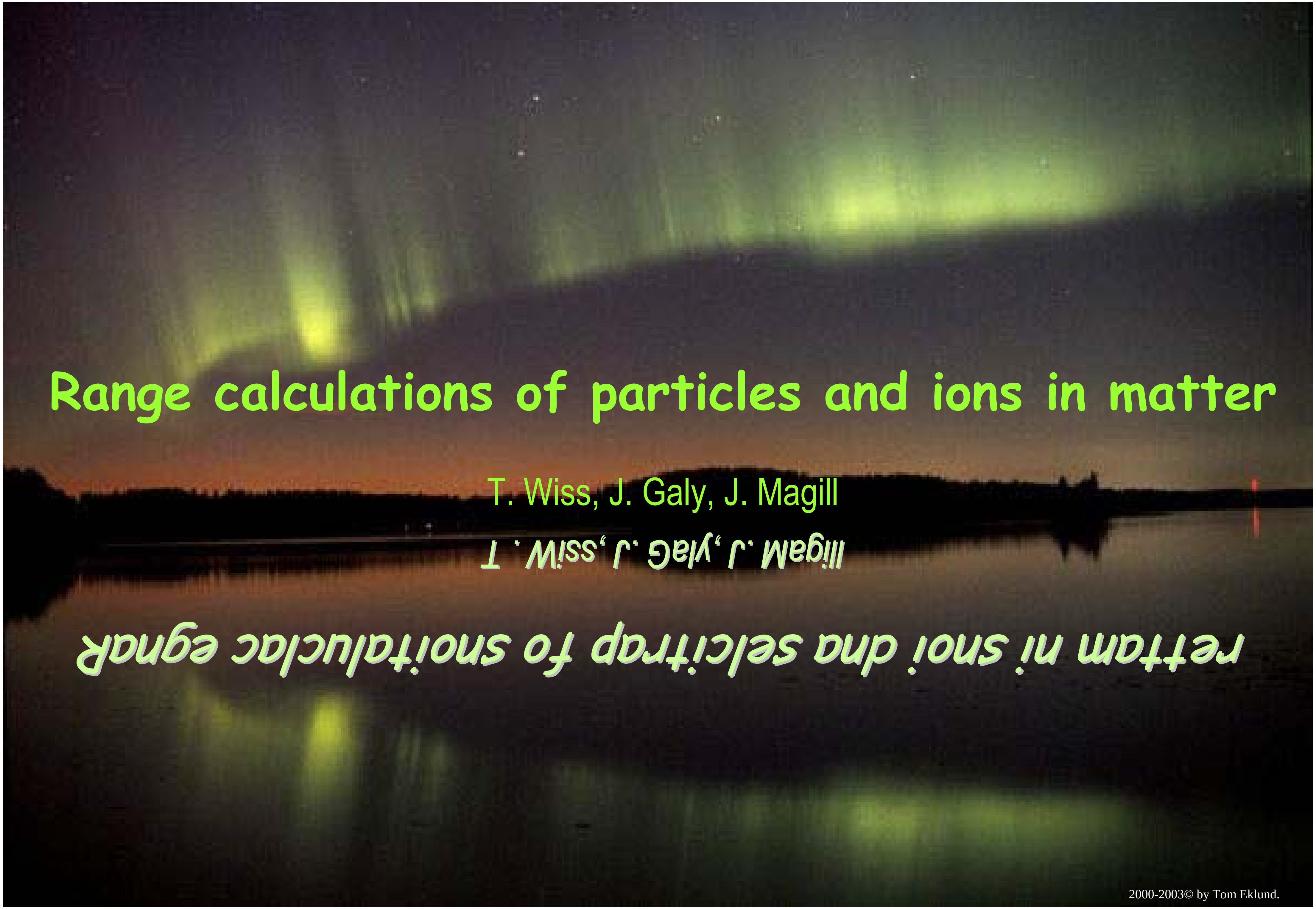

Range calculations of particles and ions in matter
T. Wiss, J. Galy, J. Magill
2000-2003© by Tom Eklund.

Content of the lecture

Introduction

Particle/ion-atom interactions
- basic processes on energy loss
- stopping power, range

Analytical approach

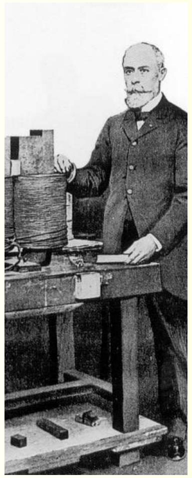
Examples

Implementation in Nuclides.net©

Joint Research Centre

Some pioneers…

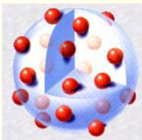
"Les rayons alpha sont des projectiles matériels susceptibles de perdre de leur vitesse en traversant la matière" (1900)

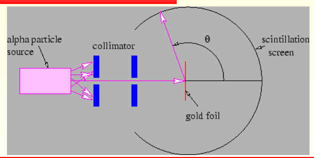


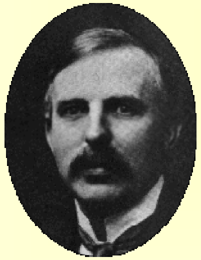
H. Becquerel

P. Curie

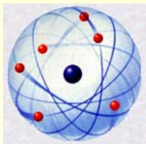
M. Curie-Slodowska







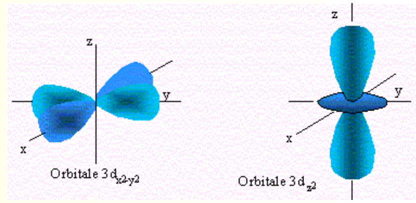
E. Rutherford

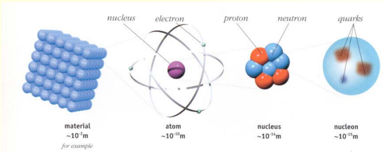


N. Bohr

E. Fermi

E. Schrödinger





1896 — 1911 — today….

itu
Institute for Transuranium Elements

Particle/ion-matter interactions

Slowing down of a particle/ion in a target

- history of the particle

  energy loss of a particle, *range*, interactions

- history of the target atoms

  displacements, recombinations, ionization, excitation, radiation damage build-up

Areas of interest

Nuclear industry, nuclear medicine, space applications, semi-conductor, geology...

Interaction of a charged particle with matter

Inelastic collisions with an electron
main process of energy loss producing excitation and ionization

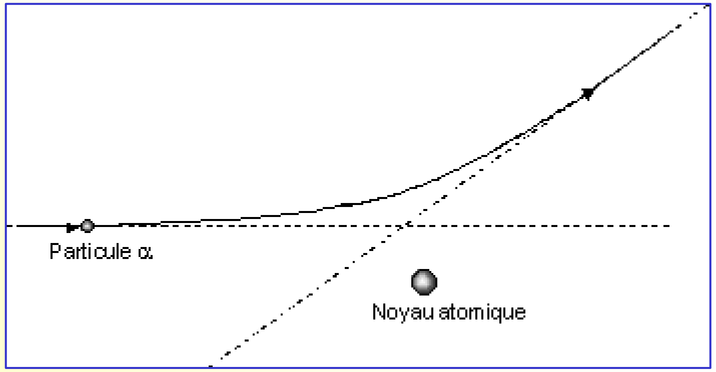
Inelastic collisions with a nucleus
Bremsstrahlung and coulombic excitation

Elastic collisions with a nucleus
Rutherford diffusion

Elastic collisions with an electron

Rutherford diffusion

$$\frac{1}{2}M_1 v_1^2 = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{D}$$



D was measured by Rutherford.
The minimum D value indicated

the upper limit of the nuclei radius.

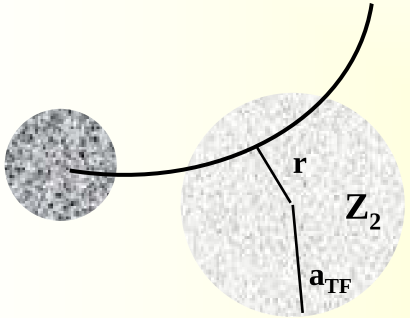
• Many interactions are needed to stop the particle (low probability of energy transfer).

• the probability to transfer energy is inverse to the mass of the target particle (mainly electrons will participate).

•Probability higher at low velocity (end of range).

….In fact..

Interatomic potential



Other description of the screening function
by Lenz, Jensen, Sommerfeld, Moliere

Inter-penetration of the electron clouds
Hartree-Fock-Slater calculations
However, good approximation by TF

Screening of e⁻ : Thomas-Fermi potential

$$V(r) = \Phi\left(\frac{r}{a_L}\right)\frac{Z_1 Z_2 e^2}{r}$$

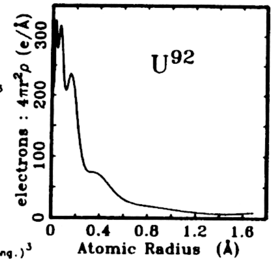
with the screening length (Lindhard)

$$a_L = \frac{0.8853}{\left(Z_1^{2/3} Z_2^{2/3}\right)^{1/2}} a_0$$

Charge distribution in single atom

U^{92}

Atomic Number 92
Atomic Weight .... 238 amu
Mass Density .... 19 g/cm³
Atomic Density .... 0.0482 Atoms/Ang.³
Lattice Type .... ORC
Lattice Constant ...... 2.85 Ang.
2nd Lattice Constant... 1.88 Ang.
Muffin-Tin Radius ..... 1.45 Ang.
Fermi Velocity-Theory (Cont).. 1.03 Vo
Fermi Velocity-Theory (Disc).. 1.01 Vo
Fermi Velocity-Experiment..... None Avail.
Interstititol Volume... 7.99 (Ang.)³
Interstitital Charge... 1.89 electrons
Interstitital Density (Disc) .. 0.236 e/(Ang.)³



Rad. (A)	Chg.(e/A³)	Rad. (A)	Chg.(e/A³)	Rad. (A)	Chg.(e/A³)	Rad. (A)	Chg.(e/A³)
0.00104	2.65E6	0.0477	9.82E3	0.255	122	1.32	0.342
0.00207	1.85E6	0.0519	8.57E3	0.272	93.3	1.45	0.246
0.00311	1.30E6	0.056	7.62E3	0.288	75.8	1.46	0.246
0.00415	9.12E5	0.0601	6.82E3	0.305	64.5	1.47	0.246
0.00519	6.47E5	0.0643	6.07E3	0.355	46.8	1.49	0.246
0.00622	4.64E5	0.0684	5.37E3	0.388	38.1	1.5	0.246
0.00726	3.40E5	0.0726	4.70E3	0.421	30	1.51	0.246
0.0083	2.54E5	0.0809	3.52E3	0.454	23	1.52	0.246
0.00933	1.96E5	0.0892	2.60E3	0.487	17.3	1.54	0.246
0.0104	1.56E5	0.0975	1.95E3	0.521	12.9	1.55	0.246
0.0124	1.10E5	0.106	1.53E3	0.554	9.68	1.56	0.246
0.0145	8.62E4	0.114	1.27E3	0.587	7.41	1.57	0.246
0.0166	7.27E4	0.122	1.11E3	0.62	5.83	1.59	0.246
0.0187	6.31E4	0.131	1.01E3	0.653	4.72	1.6	0.246
0.0207	5.51E4	0.139	9.25E2	0.72	3.33	1.61	0.246
0.0228	4.80E4	0.147	8.50E2	0.786	2.52	1.62	0.246
0.0249	4.15E4	0.156	7.75E2	0.852	1.95	1.63	0.246
0.027	3.56E4	0.172	6.17E2	0.919	1.51	1.65	0.246
0.029	3.04E4	0.189	4.65E2	0.985	1.16	1.66	0.246

Nuclear stopping power

Analytical description by Biersack $-\left.\frac{dE}{dx}\right)_n = T.d\sigma_s(E_1,T) = 4\pi N a_{TF}\left(\frac{M_1}{M_1+M_2}\right)Z_1 Z_2 e^2 \frac{\log(\varepsilon)}{2\varepsilon\left(1-\varepsilon^{-1.49}\right)}$

For ion energies below 0.1 MeV predominant process

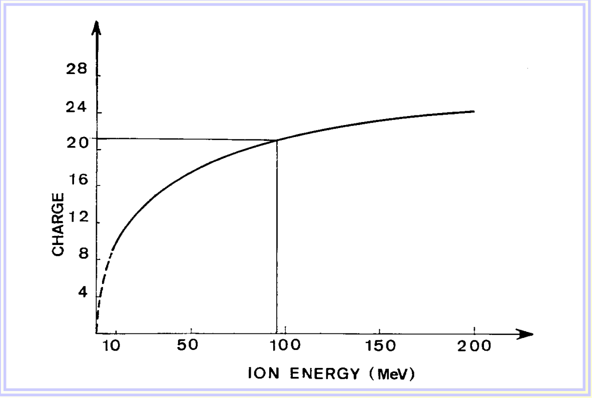
Electronic stopping power

Electronic collisions constitutes inelastic interactions where electrons can be exchanged between incident ions and target atoms. The corrected Bethe and Bloch formula is adequate for particle velocity larger than the velocity of the minimum-bound electrons.

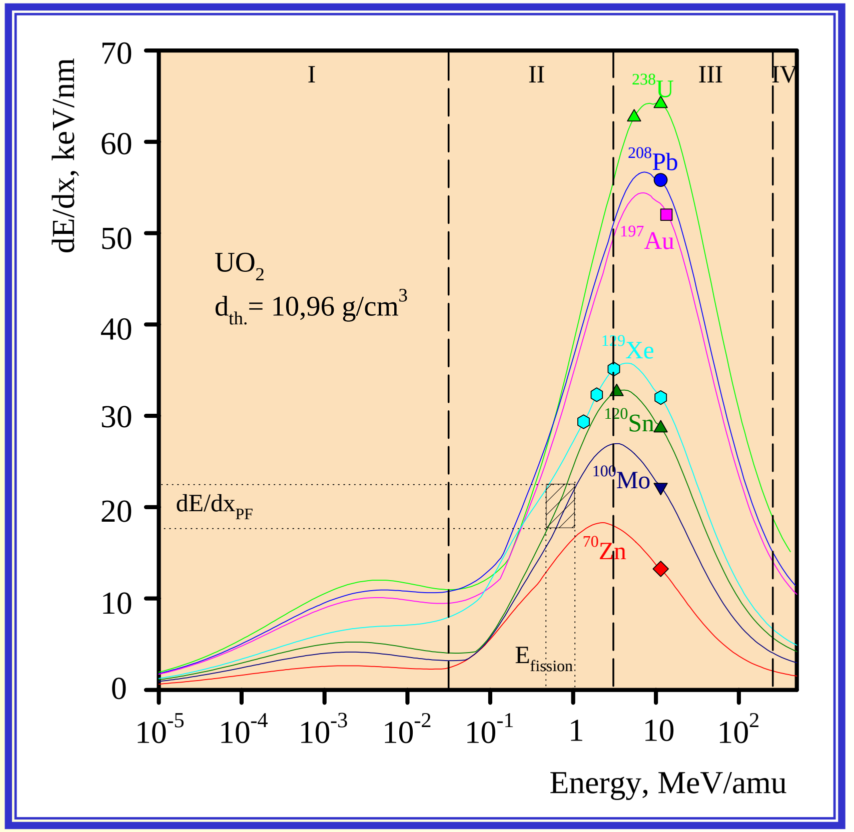
$$-\left.\frac{dE}{dx}\right)_e = nZ_2 \frac{4\pi}{m_e v_2^2}\left(\frac{Z_1^* e^2}{4\pi\varepsilon_0}\right)^2\left[\ln\left(\frac{2mv^2}{I}\right)-\beta^2-\ln\left(1-\beta^2\right)-\frac{C}{Z^2}\right]$$

For lower velocities the electron clouds can re-organize them. Lindhard and Scharff proposed an expression for the electronic stopping power based on the TF atom.

Effective charge and stopping power



Charge of a FF



Domain	Velocity
I	$v \ll Z_1 v_0$
II	$v \cong Z_1 v_0$
III	$Z_1 v_0 < v < c$
IV	$v \cong c$

v_O = Bohr velocity (electron in hydrogen) = $2.19 \cdot 10^8$ cm/s

Stopping power for electrons

For beta decays the energy distribution is a continuum with $E_{ßmax}$
Typically 2.6 keV < E < 10.4 MeV

e^- and e^+ produce ionisation and excitation along their path.
Nuclear scattering is very large

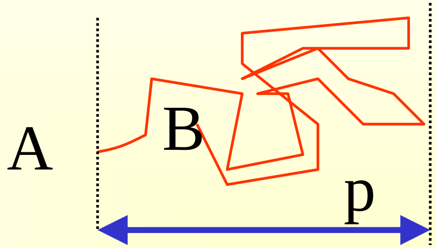
Rutherford scattering cross-section is proportional to $(M_1/m_0)^2$
$\sigma_{e-}/\sigma_{p+} = 4\ 10^6$

In fact σ can be extremely large and target e- have to be considered.

For very high energy, accelerated particles loses part of their energy radiatively as „Bremstrahlung" (govern by the Maxwell equations).
At the origin of synchrotron radiation.

Range of electrons

Difficult to assess because of the numerous scattering event (even backscattering). Rather than range, penetration depth.



Range = AB

p : penetration depth

The Z of the target has less influence since the ratio between real range and absorption thickness increases with Z but ionisation diminish.

Empirical formulation by Katz and Penfold (1952).

- 10 keV < E < 3 MeV

$R\ (mg.cm^{-2}) = 412\ E^n$ with $n = 1.265 - 0.0954 \log E$

- 1 MeV < E < 20 MeV

$R = 530\ E - 106$

Range of particles

For two particles A and B with the same velocity in the same material

$R_A = (M_A/M_B)x(Z_B/Z_A)^2 R_B$ e.g. $R_d/R_p = 2$ $R_t/R_p=3$

Rule of Bragg and Kleeman

For different materials

$R_1/R_2 = \rho_2/\rho_1 (A_1/A_2)^{1/2}$ approximation by 15%

Range of alpha-particles

Range of α in air

$E_\alpha < 4$ MeV

$R_{\alpha,air} \sim 0.56\ E_\alpha$

4MeV < E < 8 MeV

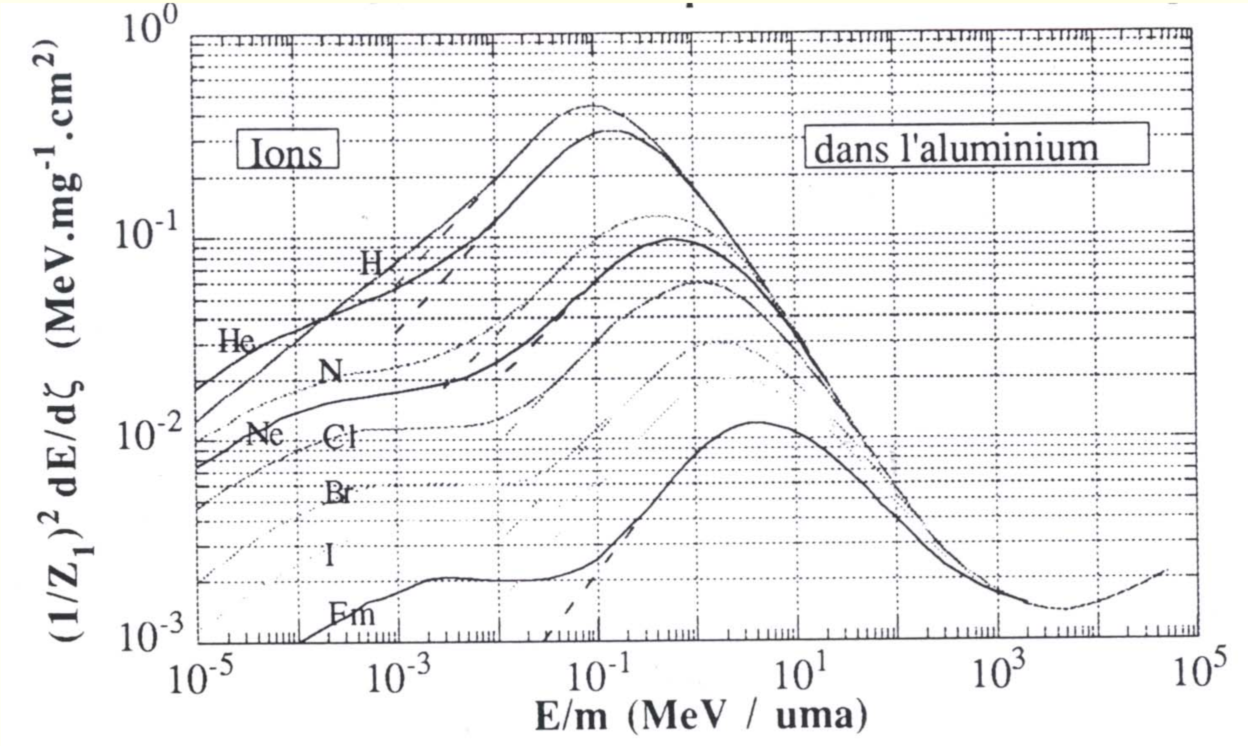
$R_{\alpha,air} \sim 1.24\ E\alpha - 2.62$

In other media

$R_\alpha \sim 5.6\ 10^{-4}\ A^{1/3}\ R_{\alpha,air}/\rho_{medium}$

Range of heavy ions

The stopping power for heavy ion can be assessed by the Bethe-Bloch approach but needs to be corrected by the effective charge (dependant on the velocity).

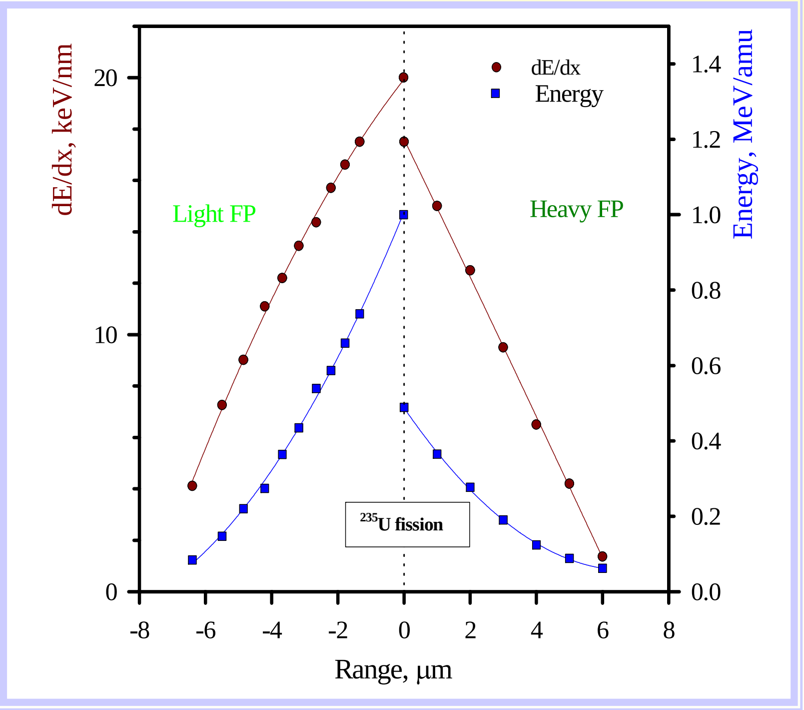


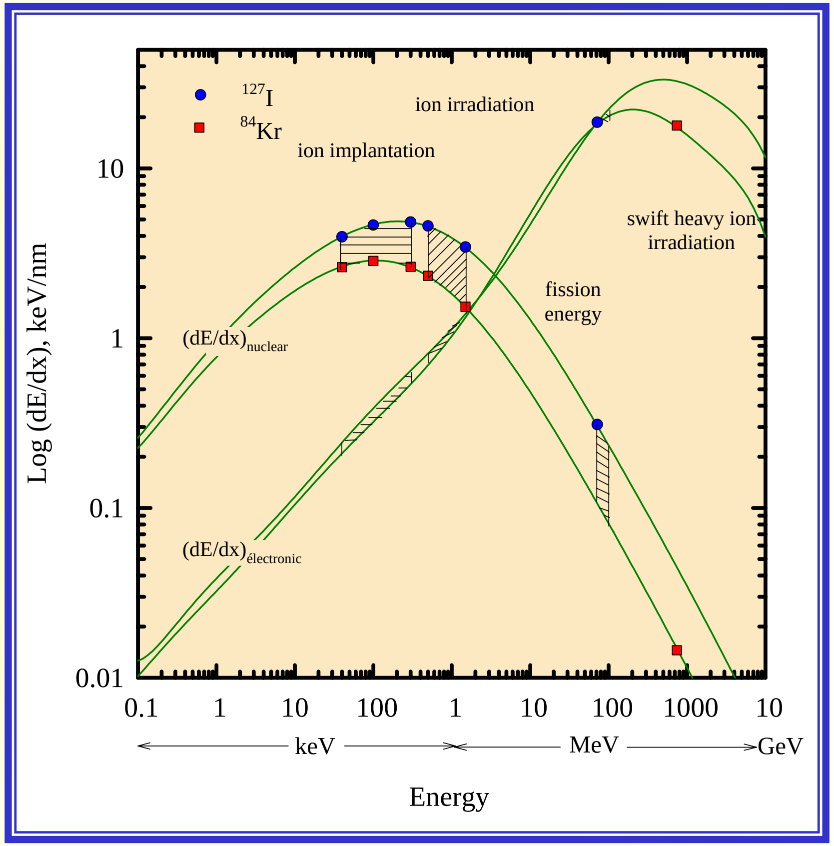
At high energy the curves of the heavy ions join the one of the proton.

From one medium to another Z/A correction.

Nuclear and Electronic stopping power and range for two fission fragments

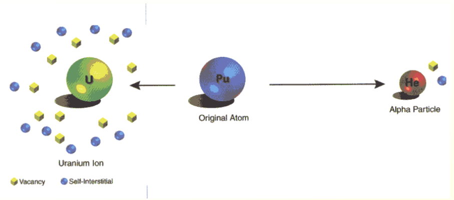
The range can be deduced from the dE/dx





Maximum $dE/dx)_n$ for 0.1 MeV
Maximum $dE/dx)_e$ for ~ 400 MeV

Range of different particles

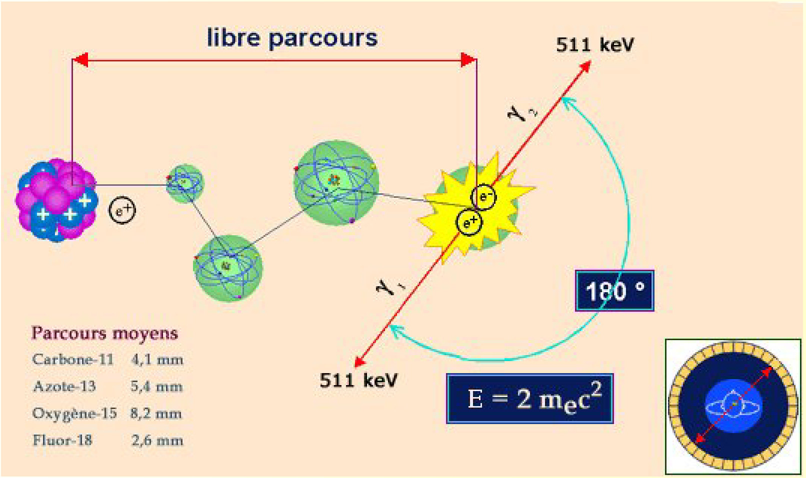


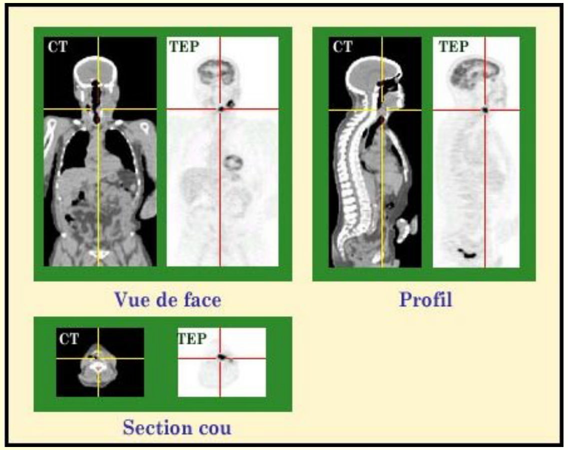
	Energy, keV	Range, µm	dE/dx, Nucl./Elec.	Defects formed
Light FPs	95000	9	0.03/0.97	40000
Heavy FPs	67000	7	0.06/0.94	60000
α-particles	5000	12	0.01/0.99	200
Recoil nucleus	95	0.02	0.90/0.10	1500
Cosmic rays (p^+)	10^{17} 10^6 (typical)	Light years !		

Particles	Origin	Use
e^-	Cosmic rays	medicine
n	Radioactivity	industry
p^+	- natural	research
d^+	- artificial	radioprotection
α	Accelerators	
heavy ions		

Positron Emission Tomography

Injection of fluorodesoxyglucose (FDG) marqued by fluor-18 allows to trace glucose consumption by tissues. This is particularly significant by cancerous tissues.

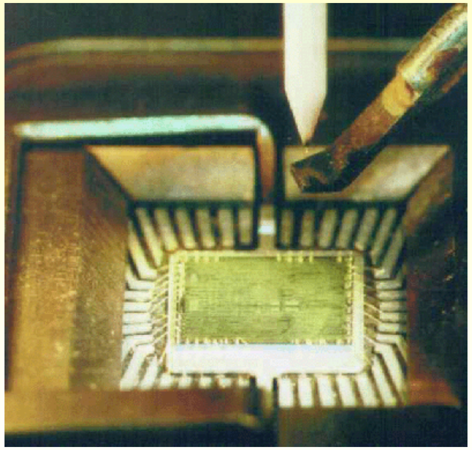




Isotope	Half live (minutes)	Emax β^+(keV)	Mean projected range (mm)
^{18}F	110	630	2,6
^{11}C	21	960	4,1
^{13}N	10	1200	5,4
^{15}O	2	1730	8,2

Junctions in semi-conductors

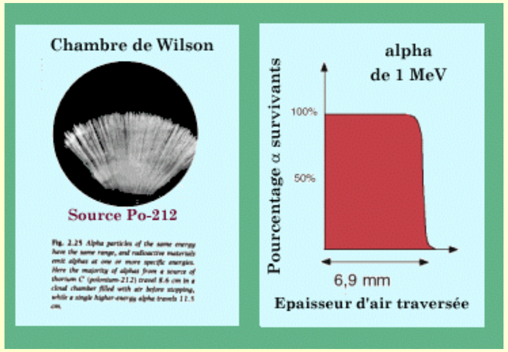
The majority of integrated circuits are fabricated from single crystal silicon wafers doped with Group III elements (B, Al, Ga, In ,Tl), p-type, or with Group V elements (N, P, As, Sb, Bi), n type. Transistors are formed by junctions between n-type and p-type silicon in the sequences n-p-n or p-n-p. Dopants are impurity elements added to the semiconductor crystal to form electrical junctions or boundaries between "n" and "p" regions in the crystal. The most common doping methods include diffusion and **ion implantation**.



Radioprotection - Shielding from radioactive sources

Joint Research Centre

- Assess the thickness of a shielding: 40 µm of Al for most of the alpha-emitters

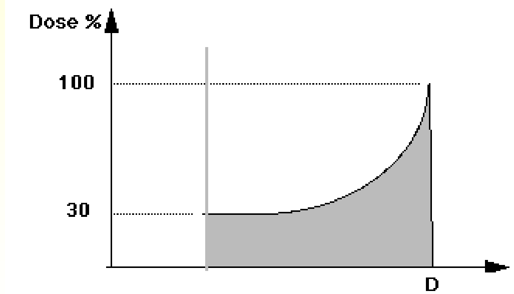


- C^{14} 0.156 MeV beta (maximum) Range 24 cm in air unshielded

Plexiglas 1 cm thick is recommended as shielding material.

- Protontherapy

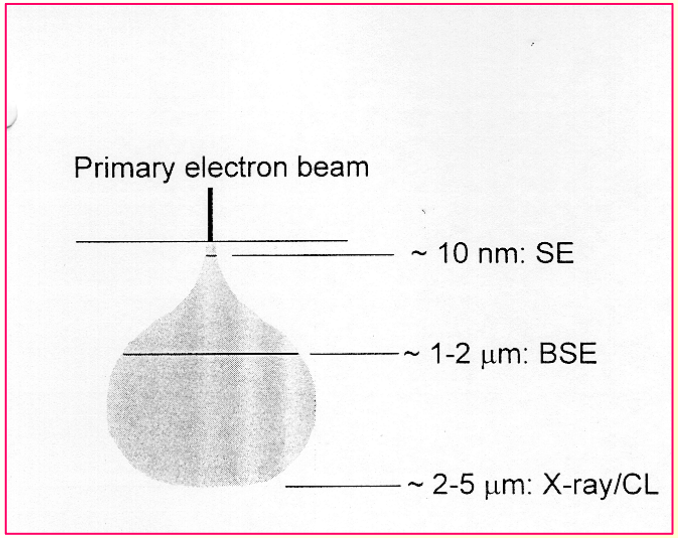
200 MeV p+ can penetrate in 22 cm tissue



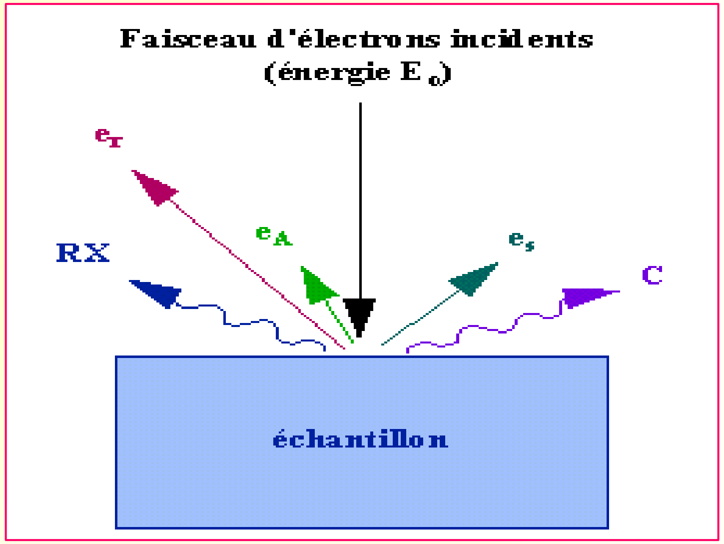
Institute for Transuranium Elements

Joint Research Centre

EDX analysis: knowing the range of electrons



e_{r}: backscattered electrons
e_{s}: secondary electrons
e_{A}: Auger electrons
RX: x-rays



Knowing the « range » of electrons helps to avoid geometrical artifacts

Database compiling stopping power and ranges

- International commission on radiation units and measurements, inc.

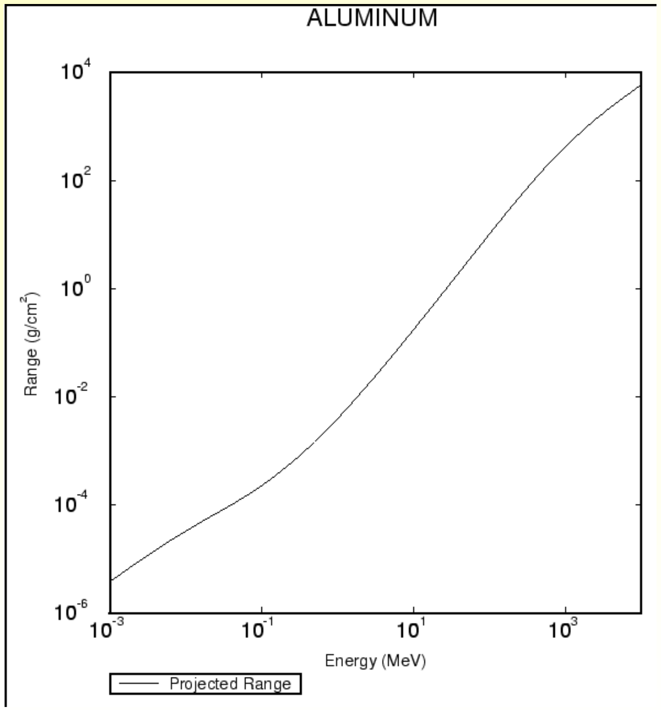
ICRU Report 49, *Stopping Power and Ranges for Protons and Alpha Particles*

- National Institute for Standards and technology, NIST

ESTAR, PSTAR, and ASTAR

estar astar pstar

Web databases ESTAR, PSTAR and ASTAR which calculate stopping powers, ranges and related quantities, for electrons, protons and helium ions. The underlying methods were developed by members of a report committee sponsored by the International Commission on Radiation Units and Measurements (ICRU).



estar astar pstar

http://physics.nist.gov/PhysRefData/Star/Text/contents.html

- ESTAR generates stopping powers and ranges for electrons which are the same as those tabulated in ICRU Report 37 (ICRU, 1984) for 72 materials at a standard grid of 81 kinetic energies between 10 keV and 1000 MeV. ESTAR can also calculate similar tables for any other element, compound or mixture. Furthermore it can calculate stopping powers at any set of kinetic energies between 1 keV and 10 GeV.

- PSTAR and ASTAR generate the stopping powers and ranges for protons and helium ions tabulated in ICRU Report 49 (ICRU, 1993) for 74 materials at a standard grid of 133 kinetic energies between 1 keV and 10 GeV for protons, and 122 kinetic energies between 1 keV and 1 GeV for helium ions. These databases can also calculate similar results at any other energy grid between these limits.

estar astar pstar

At high energies, collision stopping powers are evaluated using Bethe's stopping-power formula (Bethe, 1930). At low energies, fitting-formulas are used which are based on experimental stopping power data. The boundary between the high- and low-energy regions was at approximately 0.5 MeV for protons, and 2 MeV for alpha particles.

The details of the corrections and of the different approaches can be found n the ICRU49 report.

Range calculation in Nuclides.net©

- In most cases an estimate of the range of an electron, a particle or an ion is sufficient.

- Use of the ESTAR, PSTAR and ASTAR database.

- The stopping power and range can be accurately calculated only in defined energy ranges.